

spectrum, leaving it properly phased but inverted. This sets the phase for the f_2 dimension of the 2D.

9. Enter `wt i` to start interactive weighting. NOESY data is phase-sensitive and usually processed using Gaussian weighting, the default weighting function calculated by the setup macro. Adjust the Gaussian weighting so that data decays to zero before the end of the window. Adjusting the weighting function on the first increment of the data sets the weighting function in the 2D time dimension t_2 .
10. Enter `wft 1 da` to Fourier transform the t_2 dimension. A contour map of f_2, t_1 is displayed, showing individual interferograms. Click on trace and choose a trace through one of the interferograms. Enter `wt i` to bring up interactive weighting of the interferogram. Adjust the weighting function as before.
11. Enter `wft 2 da` to complete the Fourier transformation.
12. The f_1 dimension may now need phasing. To phase f_1 , click on trace and select a trace at the top (upfield) section of the 2D. Enter `ds` to display the trace, and phase normally using the parameter `rp`.
13. Enter `dcon 1` to redisplay the contour map with a new `rp`. Click on trace again, and select a trace at the bottom (downfield) section of the 2D. Enter `ds` and click on phase. Move the cursor upfield and click. *Do not adjust the phase at this point.* Clicking at this point sets `rp` and retains the `rp` value obtained previously. Move downfield and click. Adjust phase normally. This adjusts `lp`. Enter `dcon 1` to redisplay the properly phased 2D.
14. Enter `plcosy` to plot the data. The `plcosy` macro is general and plots all homonuclear correlated data.

Potential Problems

Unlike the COSY experiment, obtaining good NOESY spectra requires proper values of 90° pulse width and a consideration of delay times. Make sure that the 90° pulse is correct before beginning the experiment. If 90° pulse is incorrect, many "COSY type" (i.e. antiphase cross-peaks) appear, complicating the analysis. In small molecules, some "COSY-type" cross-peaks may be unavoidable even when everything is carefully calibrated. Fortunately these can be easily distinguished because of their antiphase nature, i.e., the cross-peaks have both positive and negative components but true NOE peaks are pure absorptive.

Another possible problem is the presence of artifacts due to pulsing too rapidly. Make sure you set `d1` to at least 1 to 3 times the T_1 of the protons in the sample. The NOESY experiment must be interpreted more carefully than the COSY experiment because cross-pulses arise from COSY interaction as well as dipolar interaction.

Reference

D. J. States, R. A. Haberkorn, and D. J. Ruben. *J. Magn. Reson.* **48**:286–292 (1982).

4.12 ROESY—Rotating Frame Overhauser Effect Spectroscopy

The `roesy<(ratio)>` macro sets up parameters for a ROESY pulse sequence, where the optional argument `ratio` is the desired value of the parameter `ratio` used in the sequence (`ratio` is not used in the ROESY sequence provided with *MERCURY-VX* and